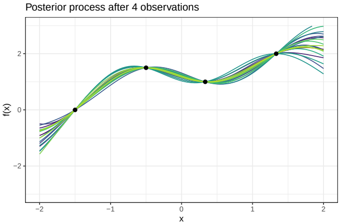
Introduction to Machine Learning

Mean Functions for Gaussian Processes



Learning goals

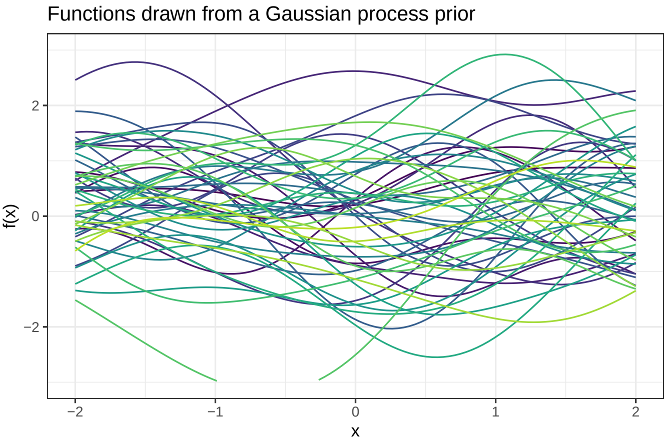
- Trends can be modeled via specification of the mean function

THE ROLE OF MEAN FUNCTIONS

- It is common but by no means necessary to consider GPs with a zero-mean function
$$m(\mathbf{x}) \equiv 0$$
- Note that this is not necessarily a drastic limitation, since the mean of the posterior process is not confined to be zero
$$\boldsymbol{f}_*|\mathbf{X}_*, \mathbf{X}, \boldsymbol{f} \sim \mathcal{N}(\mathbf{K}_*^T\mathbf{K}^{-1}\boldsymbol{f}, \mathbf{K}_{**} - \mathbf{K}_*^T\mathbf{K}^{-1}\mathbf{K}_*).$$
- Yet there are several reasons why one might wish to explicitly model a mean function, including interpretability, convenience of expressing prior informations, ...
- When assuming a non-zero mean GP prior $\mathcal{GP}\left(m(\mathbf{x}), k\left(\mathbf{x}, \mathbf{x}'\right)\right)$ with mean $m(\mathbf{x})$, the predictive mean becomes
$$m(\mathbf{X}_*) + \mathbf{K}_*\mathbf{K}_y^{-1}\left(\boldsymbol{y} - m(\mathbf{X})\right)$$
while the predictive variance remains unchanged.

THE ROLE OF MEAN FUNCTIONS

- Gaussian processes with non-zero mean Gaussian process priors are also called Gaussian processes with trend.



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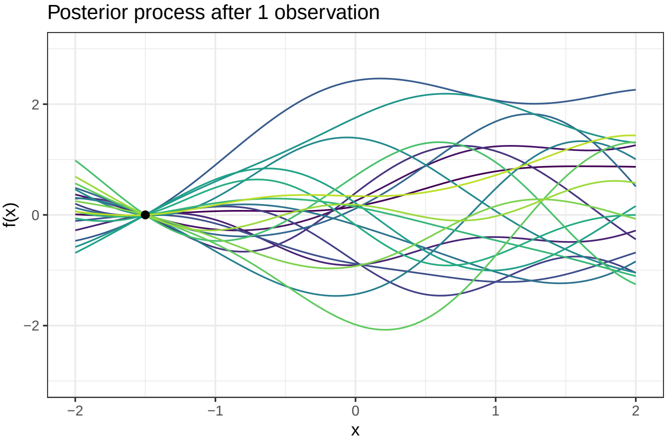

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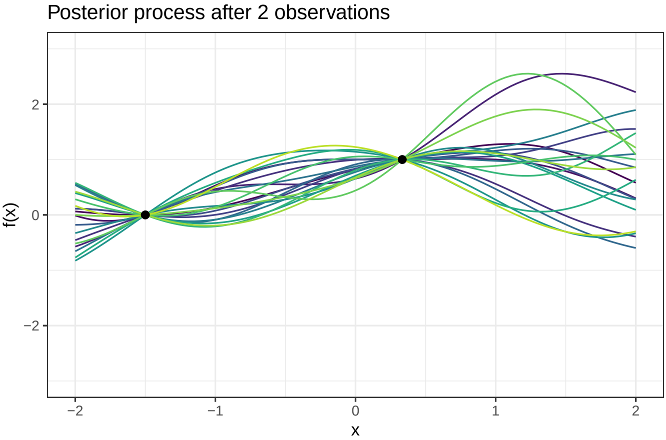

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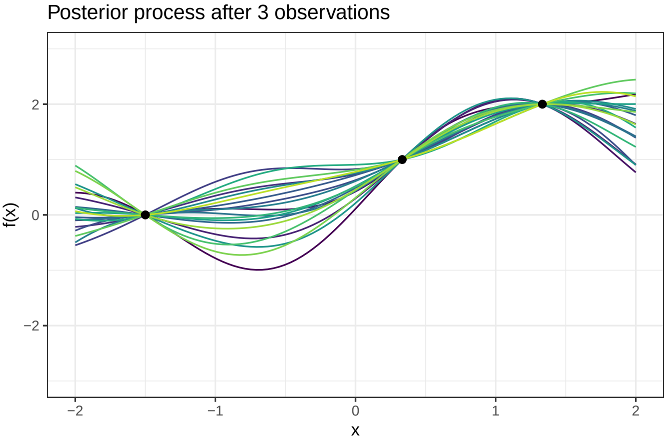

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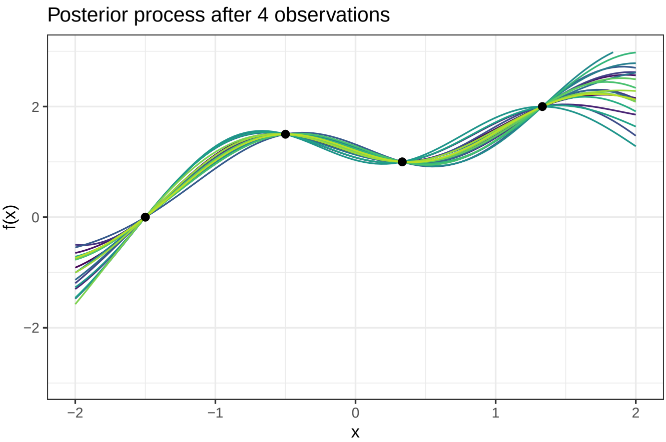

THE ROLE OF MEAN FUNCTIONS

- In practice it can often be difficult to specify a fixed mean function
- In many cases it may be more convenient to specify a few fixed basis functions, whose coefficients, β, are to be inferred from the data
- Consider

$$g(\mathbf{x}) = b(\mathbf{x})^\top \beta + f(\mathbf{x}), \text{ where } f(\mathbf{x}) \sim \mathcal{GP}\left(0, k(\mathbf{x}, \tilde{\mathbf{x}})\right)$$

- This formulation expresses that the data is close to a global linear model with the residuals being modelled by a GP.
- For the estimation of $g(\mathbf{x})$ please refer to *Rasmussen, Gaussian Processes for Machine Learning, 2006*